Figure S1 Correlation chord diagrams on differential metabolites.

STEMI-CONTROL

NSTEMI-CONTROL

UA-CONTROL

STEMI-NSTEMI
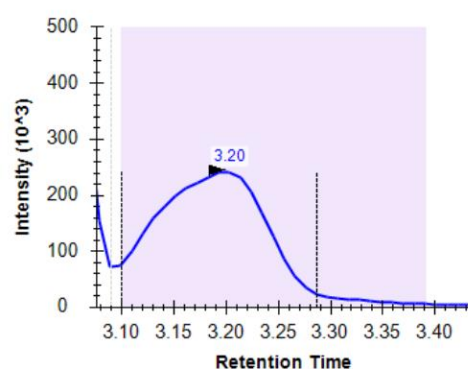
STEMI-UA

NSTEMI-UA
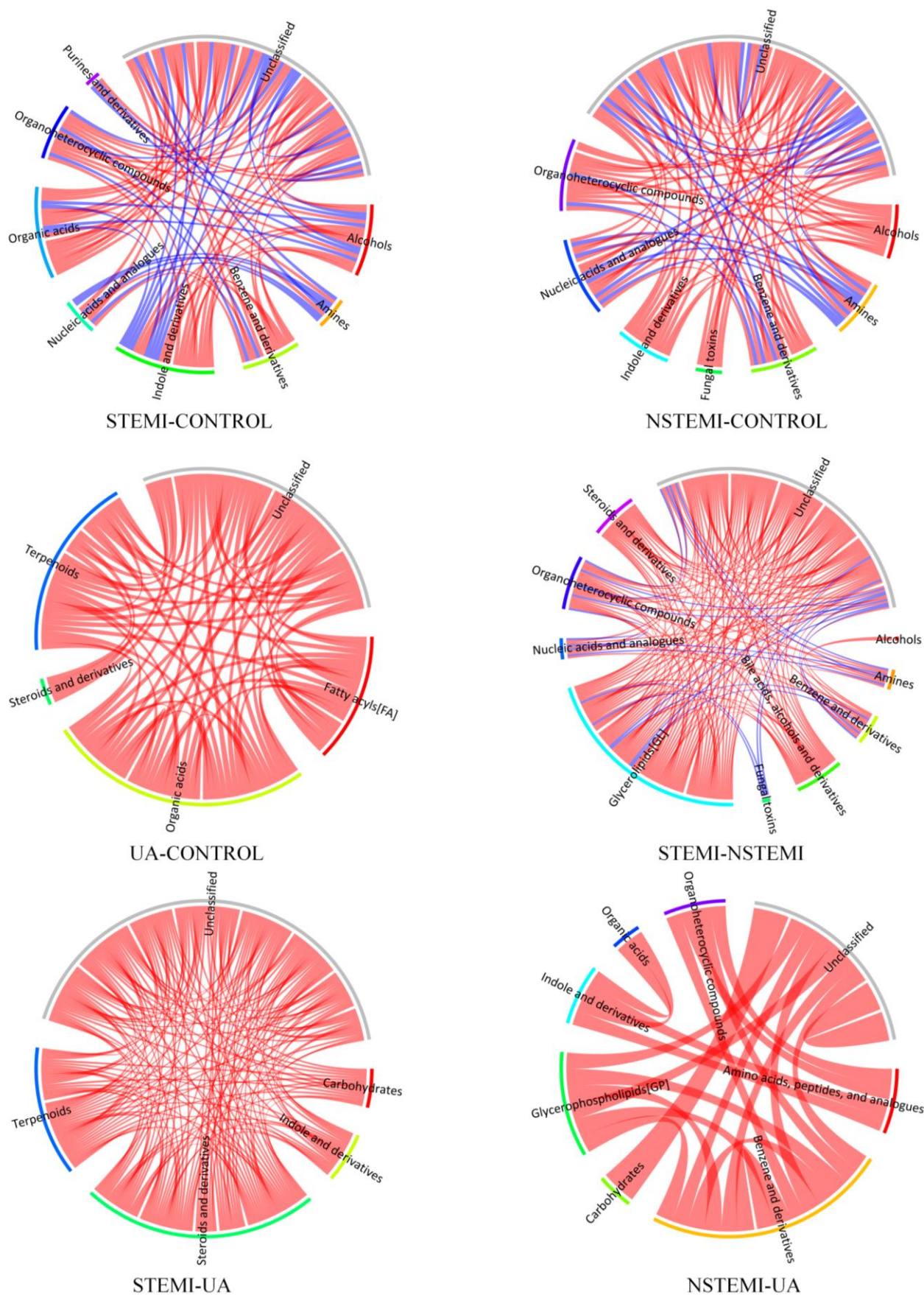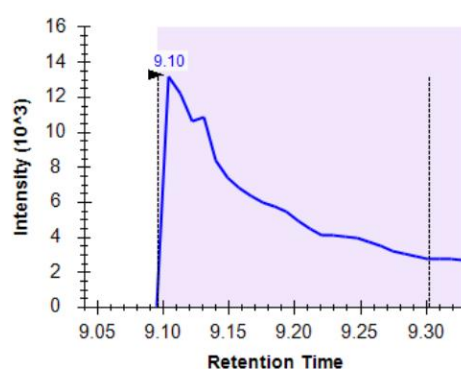
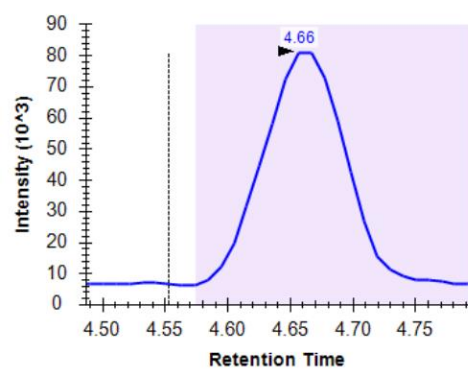**Figure S2** Mass spectra of 14 differential metabolites.
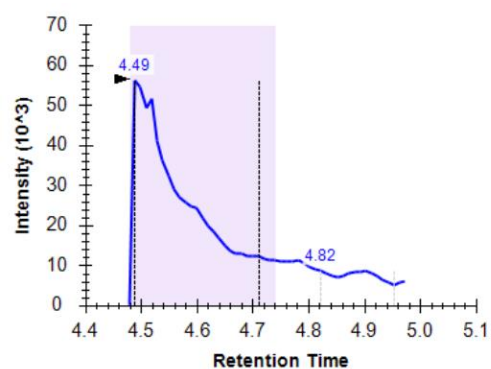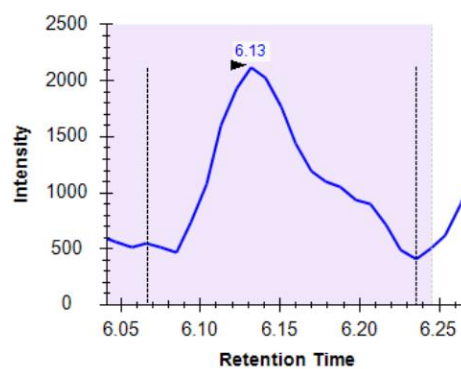

L-Aspartic acid
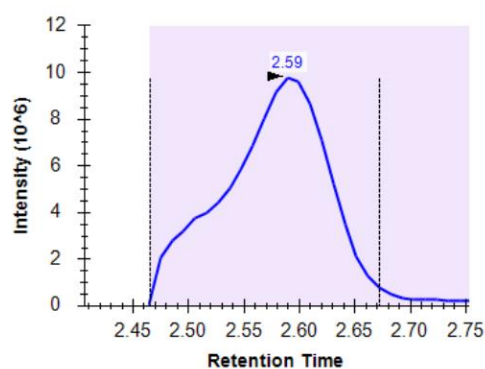
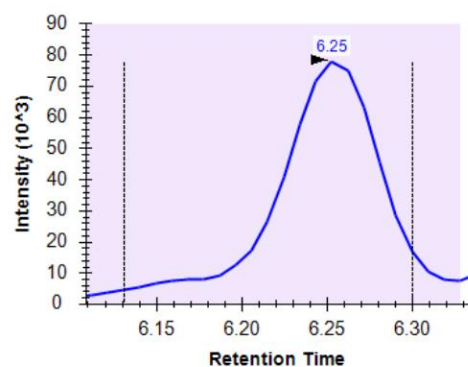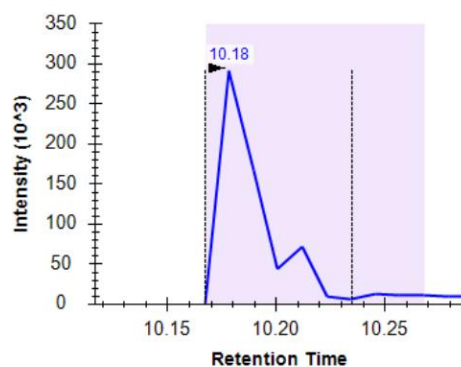L-Acetylcarnitine

Acetylglycine

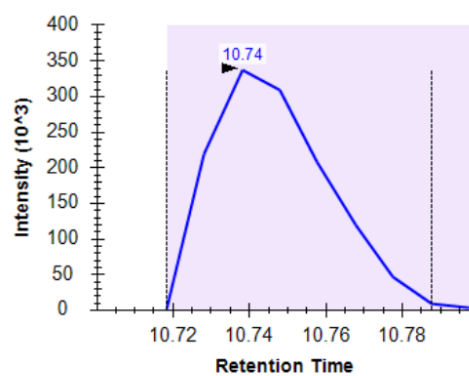Decanoylcarnitine (C10)
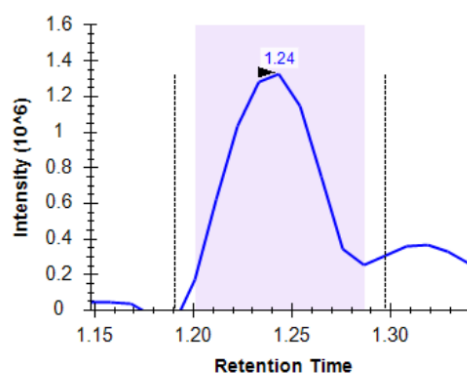
Hydroxyphenyllactic acid

Ferulic acid

Itaconic acid

Lauroylcarnitine

Figure S2 Continued

Myristoylcarnitine

cis-4-Hydroxy-D-proline
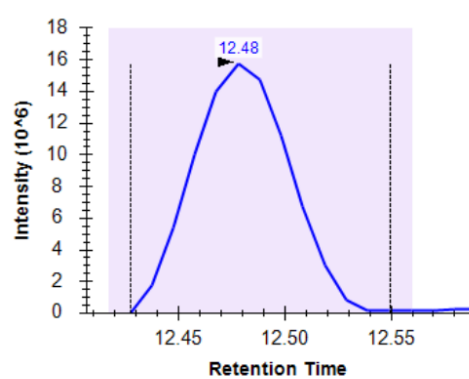
Arachidonic acid
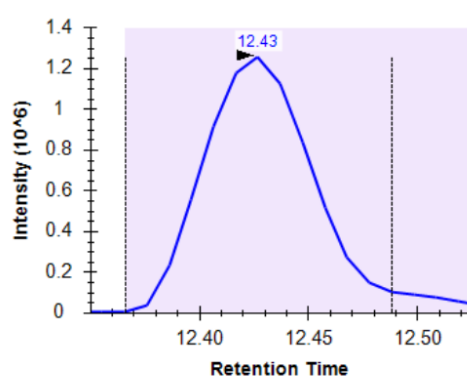
Palmitoleic acid
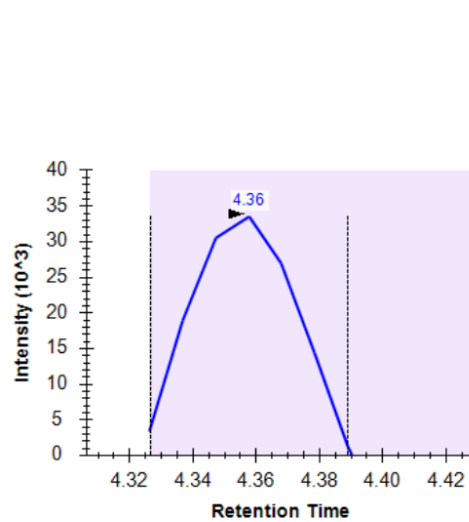
D-Aspartic acid
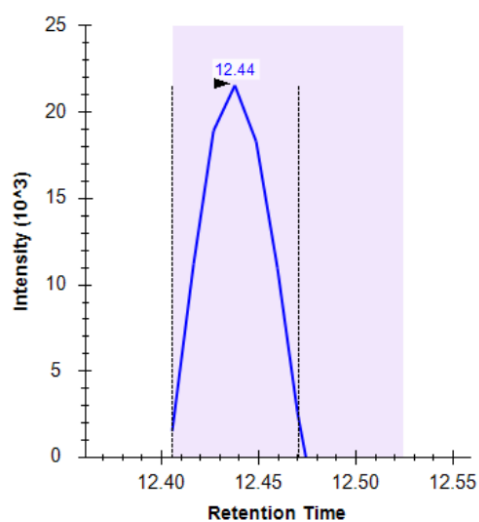
Palmitelaidic acid

Table S1 Multiple hypothesis test of factors with significant differences.

	group I	group J	p-adjusted
Cardiac Biomarkers			
	STEMI	NSTEMI	0.579
Myo	STEMI	UA	<0.001
	NSTEMI	UA	0.006
	STEMI	NSTEMI	1.000
CKMB	STEMI	UA	0.002
	NSTEMI	UA	0.005
	STEMI	NSTEMI	1.000
TnI	STEMI	UA	0.017
	NSTEMI	UA	0.002
Laboratory data			
	control	STEMI	<0.001
	control	NSTEMI	<0.001
	control	UA	0.014
Blood glucose	STEMI	NSTEMI	1.000
	STEMI	UA	0.972
	NSTEMI	UA	1.000
	control	STEMI	0.017
	control	NSTEMI	1.000
	control	UA	1.000
ALT	STEMI	NSTEMI	0.004
	STEMI	UA	0.001
	NSTEMI	UA	1.000
	control	STEMI	<0.001
	control	NSTEMI	0.017
	control	UA	1.000
AST	STEMI	NSTEMI	0.06
	STEMI	UA	<0.001
	NSTEMI	UA	0.014
	control	STEMI	<0.001
	control	NSTEMI	<0.001
	control	UA	1.000
ALT/AST	STEMI	NSTEMI	0.681
	STEMI	UA	<0.001
	NSTEMI	UA	0.035
	control	STEMI	0.166
	control	NSTEMI	0.175
TP	control	UA	0.028
	STEMI	NSTEMI	1.000

	STEMI	UA	1.000
	NSTEMI	UA	1.000
	control	STEMI	0.538
	control	NSTEMI	0.216
TG	control	UA	0.030
	STEMI	NSTEMI	1.000
	STEMI	UA	1.000
	NSTEMI	UA	1.000
	control	STEMI	0.665
	control	NSTEMI	0.008
HDL-C	control	UA	0.006
	STEMI	NSTEMI	0.137
	STEMI	UA	0.084
	NSTEMI	UA	0.967

Length of stay

	control	STEMI	<0.001
	control	NSTEMI	<0.001
	control	UA	0.101
	STEMI	NSTEMI	1.000
	STEMI	UA	0.032
	NSTEMI	UA	0.169

Table S2 Summary of DMs pathways of discovery phase.

Group	TOP3 pathway	DMs number	TOP1 DMs proportion pathway	TOP1 DMs number pathway
	Neuroactive ligand-receptor interaction（hsa04080）	7		
STEMI-CTRL	Retrograde endocannabinoid signaling（hsa04723）	5	Retrograde endocannabinoid signaling（hsa04723）	Steroid hormone biosynthesis（hsa00140）
	Steroid hormone biosynthesis（hsa00140）	8		
	Biosynthesis of unsaturated fatty acids（hsa01040）	8		
NSTEMI-CTRL	Linoleic acid metabolism（hsa00591）	5	Retrograde endocannabinoid signaling（hsa04723）	Biosynthesis of unsaturated fatty acids（hsa01040）
	Retrograde endocannabinoid signaling（hsa04723）	4		
	Biosynthesis of unsaturated fatty acids（hsa01040）	13		
UA-CTRL	Linoleic acid metabolism（hsa00591）	6	Fc gamma R-mediated phagocytosis（hsa04666）	Biosynthesis of unsaturated fatty acids（hsa01040）
	Neuroactive ligand-receptor interaction（hsa04080）	6		
	Cholesterol metabolism（hsa04979）	2	Prion diseases（hsa05020）	
STEMI-NSTEMI	Steroid hormone biosynthesis（hsa00140）	4		Steroid hormone biosynthesis（hsa00140）
	Taurine and hypotaurine metabolism（hsa00430）	2	Huntington disease（hsa05016）	
	Protein digestion and absorption（hsa04974）	7		Protein digestion and absorption（hsa04974）
STEMI-UA	Steroid hormone biosynthesis（hsa00140）	7	FoxO signaling pathway（hsa04068）	
	Aminoacyl-tRNA biosynthesis（hsa00970）	5		Steroid hormone biosynthesis（hsa00140）
	Protein digestion and absorption（hsa04974）	7		
NSTEMI-UA	ABC transporters（hsa02010）	8	Amyotrophic lateral sclerosis (ALS)（hsa05014）	ABC transporters（hsa02010）
	Aminoacyl-tRNA biosynthesis（hsa00970）	6		

Table S3 Summary of DMs pathways of validation phase.

Group	TOP3 pathway	DMs number	TOP1 DMs proportion pathway	TOP1 DMs number pathway
	Central carbon metabolism in cancer（hsa05230）	6		
STEMI-CTRL	Biosynthesis of amino acids（hsa01230）	8	Arginine biosynthesis（hsa00220）	Biosynthesis of amino acids（hsa01230）
	Arginine biosynthesis（hsa00220）	5		
	Biosynthesis of unsaturated fatty acids（hsa01040）	6		Biosynthesis of unsaturated fatty acids（hsa01040）
NSTEMI-CTRL	Biosynthesis of amino acids（hsa01230）	6	Arginine biosynthesis（hsa00220）	Biosynthesis of amino acids（hsa01230）
	Arginine biosynthesis（hsa00220）	4		
	Biosynthesis of unsaturated fatty acids（hsa01040）	3		Biosynthesis of unsaturated fatty acids（hsa01040）
STEMI-NSTEMI	ABC transporters（hsa02010）	3	Renal cell carcinoma（hsa05211）	ABC transporters（hsa02010）
	Central carbon metabolism in cancer（hsa05230）	2		

Table S4 Regression analysis of DMs and CKMB.

		CKMB	
		P	Coefficients
STEMI	L-Aspartic acid	0.002	1.893
	L-Acetylcarnitine	0.001	3.121
	Acetylglycine	1.000	-
	Decanoylcarnitine	0.287	-
	Hydroxyphenyllactic acid	0.295	-
	Ferulic acid	0.793	-
	Itaconic acid	0.175	-
	Lauroylcarnitine	0.082	-
	Myristoylcarnitine	0.013	0.001
	cis-4-Hydroxy-D-proline	0.188	-
	L-Aspartic acid	0.291	-
	Arachidonic acid	0.391	-
NSTEMI	Palmitoleic acid	0.526	-
	D-Aspartic acid	0.438	-
	Palmitelaidic acid	0.494	-

Table S5 Regression analysis of DMs and disease severity.

		P value severity
STEMI	L-Aspartic acid	All the samples were multi-vessel diseases, and there was no difference in severity.
	L-Acetylcarnitine	
	Acetylglycine	
	Decanoylcarnitine	
	Hydroxyphenyllactic acid	
	Ferulic acid	
	Itaconic acid	
	Lauroylcarnitine	
	Myristoylcarnitine	
	cis-4-Hydroxy-D-proline	
NSTEMI	L-Aspartic acid	0.397
	Arachidonic acid	0.893
	Palmitoleic acid	0.473
	D-Aspartic acid	0.266
	Palmitelaidic acid	0.391

Table S6 Regression analysis of DMs and risk factors.

		P value			
		Hypertension	Diabetes	Dyslipidemia	Smoke
STEMI	L-Aspartic acid	0.382	0.476	0.334	0.438
	L-Acetylcarnitine	0.432	0.840	0.598	0.504
	Acetylglycine	0.801	0.970	0.824	0.760
	Decanoylcarnitine	0.665	0.431	0.984	0.740
	Hydroxyphenyllactic acid	0.002	0.002	0.002	0.007
	Ferulic acid	0.673	0.582	0.618	0.665
	Itaconic acid	0.198	0.597	0.558	0.648
	Lauroylcarnitine	0.468	0.552	0.773	0.965
	Myristoylcarnitine	0.373	0.848	0.570	0.909
	cis-4-Hydroxy-D-proline	0.271	0.273	0.095	0.115
	L-Aspartic acid	0.485	0.472	0.716	0.791
	Arachidonic acid	0.792	0.675	0.603	0.723
NSTEMI	Palmitoleic acid	0.998	0.674	0.839	0.171
	D-Aspartic acid	0.509	0.476	0.886	0.931
	Palmitelaidic acid	0.844	0.601	0.666	0.196